Anisotropic Plasticity of NiAl under Dynamical Loading

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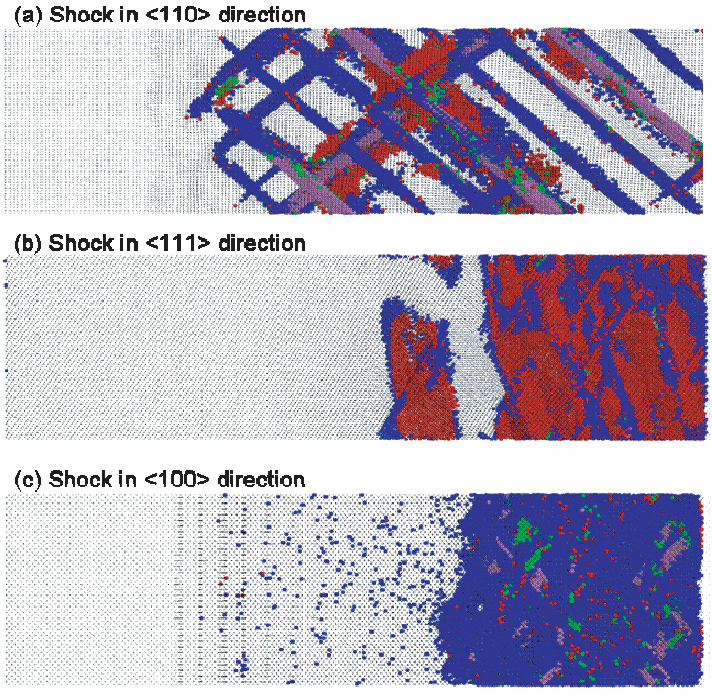
Ordered intermetallic alloys have attracted significant attention due to their potential application as structural materials in high temperature environments. NiAl, a metallic alloy with the B2 crystal structure, is among the most promising materials for such applications due to its low density, high melting temperature (1912 K) and excellent corrosion resistance. However, NiAl suffers from poor ductility at room temperature and its mechanisms of plastic deformation are poorly characterized. An atomic-level understanding of plasticity in B2 metallic alloys is a critical step towards the development of new alloys with optimized properties.

We use molecular dynamics (MD) with an accurate interatomic potential to study the mechanical response of NiAl when shocked along <110>, <111>, and <100> directions. For strong enough shockwaves, plastic deformation relaxes the uniaxial compression of the shock; we focus on this relaxation phenomenon.

Figure 1 shows snapshots from our simulations. We color atoms according to the plastic slip they have undergone: blue atoms have slipped by 1/2*a*<111>, purple ones have done so by *a*<111>, red by *a*<100>, and green by *a*<110> (where *a* is the lattice parameter); elastically deformed and unshocked atoms are shown as small black dots.

Our results show that for shocks in the <110> direction, the first event regarding plastic deformation is the nucleation of 1/2<111> loops (blue atoms); the edge components of these loops move toward and away from the shock front. The B2 lattice is not invariant against translations by 1/2*a*<111>; thus, the area swept by these loops is left defective [with an antiphase defect (AFD)] and their growth is energetically unfavorable. Thus, a second 1/2<111> loop is nucleated inside the original ones leading to <111> slip



MD snapshots of shock wave propagation in NiAl in the <110>, <111>, and <100> directions.

Figure 1—
The figure shows snapshots from our simulations. We color atoms according to the plastic slip they have undergone: blue atoms have slipped by 1/2a<111>, purple ones have done so by a<111>, red by a<100> and green by a<110> (where a is the lattice parameter); elastically deformed and unshocked atoms are shown as small black dots.

(purple atoms). At later times we observe the nucleation of <100> slip, predominantly at the intersection of 1/2<111> loops. We find that the plastic wave moves at the same speed of the shock front. For shocks in the <111> direction plastic deformation also begins with the nucleation of 1/2<111> loops, but in this case the nucleation of the second 1/2*a*<111> loops inside the original ones lead to <100> slip (red atoms). In this case, the plastic wave does not catch up with the shock front: the plastic wave propagates slower that the shockwave and an elastic precursor develops. Finally, for loading in the <100> direction we observe multiple, almost simultaneous, nucleation of 1/2<111> loops and the frequent intersection thereof; this entanglement severely limits their mobility and even leads to local amorphization.

In summary, we used MD simulations to characterize the details of the plastic response of NiAl single crystals under compressive uniaxial loading. While in all cases plastic deformation starts with the nucleation of 1/2*a*<111> loops, the subsequent phenomena exhibits marked anisotropy. Shocks in <110> have a single wave structure with the plastic wave traveling at the shock speed; on the other hand for <111> and <100> loading we find a two-wave structure with the plastic wave following an elastic precursor.

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